NUCLEAR ENERGY RESEARCH INITIATIVE

Multi-scale Modeling of the Deformation of Advanced Ferritic Steels for Generation IV Nuclear Energy Systems

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Program Area: Generation IV

Project Description

This project will use the Multi-scale Modeling of Materials (MMM) approach to develop an improved understanding of the effects of neutron irradiation on the mechanical properties of high-temperature materials (i.e., 650-700°C, compared to the current 550°C limit). Presently, there are no physically-based models for high-temperature, in-reactor, deformation of advanced ferritic/martensitic steels. The objective of this project is to develop such a model.

Empirical potentials are not well developed for alloys and cannot easily adapt to local changes in chemistry caused by impurities. In this project, *ab-initio* calculations will be combined with traditional Molecular Dynamics (MD) simulations of dislocation-defect interactions. Particular emphasis will be placed on determining interactions with oxide and carbide precipitates, which control the ductility and high-temperature strength of steels, and on simulating properties of radiation-damaged steels as a function of neutron dose. The analysis will also determine interaction with nano-voids, precipitates, and self-interstitial clusters during irradiation. This information will be used to enhance a comprehensive model of radiation damage and in-reactor deformation. Predictions will be made for in-reactor deformation of simplified geometry, with full microstructure information linked with the deformation field.

Workscope

The following key activities comprise the project workscope:

- Develop and test the hybrid atomistic-continuum model for bcc metals
- Apply the approach to study dislocation in a pure alloy (Fe-Cr) host
- Perform simulations of interaction mechanisms and determine stress relationships
- Extend model to twin boundaries and study dislocation properties in Fe-Cr alloys
- Evaluate effect of H, He, and C on properties and continue simulations to determine suitable rate theory parameters
- Apply to other materials and extend models
- Compare Rate Theory model with experimental data and model Generation IV vessel sections